# Kasper P. Kepp

List of Publications by Year
in descending order



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|---|---|---|---|
| 132 papers | 6,567 citations | 70961 41 h-index | 76769 74 g-index |
| 140 all docs | 140 docs citations | 140 times ranked | 7265 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Bioinorganic Chemistry of Alzheimerâ€™s Disease. Chemical Reviews, 2012, 112, 5193-5239. | 23.0 | 581 |
| 2 | A Quantitative Scale of Oxophilicity and Thiophilicity. Inorganic Chemistry, 2016, 55, 9461-9470. | 1.9 | 360 |
| 3 | Halide, Ammonium, and Alkali Metal Ion Parameters for Modeling Aqueous Solutions. Journal of Chemical Theory and Computation, 2006, 2, 1499-1509. | 2.3 | 355 |
| 4 | Performance of density functionals for first row transition metal systems. Journal of Chemical Physics, 2007, 126, 014103. | 1.2 | 210 |
| 5 | Consistent descriptions of metalâ€“ligand bonds and spin-crossover in inorganic chemistry. Coordination Chemistry Reviews, 2013, 257, 196-209. | 9.5 | 172 |
| 6 | How O2 Binds to Heme. Journal of Biological Chemistry, 2004, 279, 14561-14569. | 1.6 | 170 |
| 7 | Theoretical Prediction of the Coâ€“C Bond Strength in Cobalamins. Journal of Physical Chemistry A, 2003, 107, 7539-7545. | 1.1 | 168 |
| 8 | Bioinorganic Chemistry Modeled with the TPSSh Density Functional. Inorganic Chemistry, 2008, 47, 10357-10365. | 1.9 | 146 |
| 9 | Theoretical Study of Spin Crossover in 30 Iron Complexes. Inorganic Chemistry, 2016, 55, 2717-2727. | 1.9 | 139 |
| 10 | Accurate Computed Enthalpies of Spin Crossover in Iron and Cobalt Complexes. Journal of Physical Chemistry A, 2009, 113, 10033-10039. | 1.1 | 138 |
| 11 | Metal Ion Enhanced Binding of AMD3100 to Asp262in the CXCR4 Receptorâ€. Biochemistry, 2003, 42, 710-717. | 1.2 | 134 |
| 12 | Alzheimerâ€™s disease: How metal ions define Î²-amyloid function. Coordination Chemistry Reviews, 2017, 351, 127-159. | 9.5 | 120 |
| 13 | How the Coâ€“C Bond Is Cleaved in Coenzyme B12Enzymes:Â A Theoretical Study. Journal of the American Chemical Society, 2005, 127, 9117-9128. | 6.6 | 118 |
| 14 | Alzheimerâ€™s disease due to loss of function: A new synthesis of the available data. Progress in Neurobiology, 2016, 143, 36-60. | 2.8 | 111 |
| 15 | The Dependence of Amyloidâ€Î²2 Dynamics on Protein Force Fields and Water Models. ChemPhysChem, 2015, 16, 3278-3289. | 1.0 | 103 |
| 16 | O-binding to heme: electronic structure and spectrum of oxyheme, studied by multiconfigurational methods. Journal of Inorganic Biochemistry, 2005, 99, 45-54. | 1.5 | 97 |
| 17 | Characterization of an Alkali- and Halide-Resistant Laccase Expressed in E. coli: CotA from Bacillus clausii. PLoS ONE, 2014, 9, e99402. | 1.1 | 97 |
| 18 | The Chemical Bond between Transition Metals and Oxygen: Electronegativity, d-Orbital Effects, and Oxophilicity as Descriptors of Metalâ€“Oxygen Interactions. Journal of Physical Chemistry C, 2019, 123, 18432-18444. | 1.5 | 92 |

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| 19 | A structural-chemical explanation of fungal laccase activity. Scientific Reports, 2018, 8, 17285. | 1.6 | 89 |
| 20 | Accurate Stabilities of Laccase Mutants Predicted with a Modified FoldX Protocol. Journal of Chemical Information and Modeling, 2012, 52, 3028-3042. | 2.5 | 80 |
| 21 | Spin Propensities of Octahedral Complexes From Density Functional Theory. Journal of Physical Chemistry A, 2015, 119, 4041-4050. | 1.1 | 80 |
| 22 | Iron(II) and Iron(III) Spin Crossover: Toward an Optimal Density Functional. Journal of Physical Chemistry A, 2018, 122, 4208-4217. | 1.1 | 79 |
| 23 | Polarization Effects for Hydrogen-Bonded Complexes of Substituted Phenols with Water and Chloride Ion. Journal of Chemical Theory and Computation, 2007, 3, 1987-1992. | 2.3 | 73 |
| 24 | Comment on â€œDensity functional theory is straying from the path toward the exact functionalâ€• Science, 2017, 356, 496-496. | 6.0 | 72 |
| 25 | Ten Challenges of the Amyloid Hypothesis of Alzheimerâ€™s Disease. Journal of Alzheimer's Disease, 2016, 55, 447-457. | 1.2 | 71 |
| 26 | Comparison of the Chemical Properties of Iron and Cobalt Porphyrins and Corrins. ChemBioChem, 2003, 4, 413-424. | 1.3 | 66 |
| 27 | Copper imbalance in Alzheimerâ€™s disease: Convergence of the chemistry and the clinic. Coordination Chemistry Reviews, 2019, 397, 168-187. | 9.5 | 65 |
| 28 | The axial N -base has minor influence on Coâ€“C bond cleavage in cobalamins. Computational and Theoretical Chemistry, 2002, 585, 239-255. | 1.5 | 64 |
| 29 | Chemical Bond Energies of 3d Transition Metals Studied by Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 3479-3492. | 2.3 | 64 |
| 30 | Cobalamins uncovered by modern electronic structure calculations. Coordination Chemistry Reviews, 2009, 253, 769-778. | 9.5 | 61 |
| 31 | The role of axial ligands for the structure and function of chlorophylls. Journal of Biological Inorganic Chemistry, 2006, 12, 49-61. | 1.1 | 59 |
| 32 | Theoretical Investigation of Steric and Electronic Effects in Coenzyme B12Models. Organometallics, 2001, 20, 550-556. | 1.1 | 58 |
| 33 | Membrane Dynamics of Î³-Secretase Provides a Molecular Basis for Î²-Amyloid Binding and Processing. ACS Chemical Neuroscience, 2017, 8, 2424-2436. | 1.7 | 54 |
| 34 | Positively Selected Sites in Cetacean Myoglobins Contribute to Protein Stability. PLoS Computational Biology, 2013, 9, e1002929. | 1.5 | 52 |
| 35 | The dynamic mechanism of presenilin-1 function: Sensitive gate dynamics and loop unplugging control protein access. Neurobiology of Disease, 2016, 89, 147-156. | 2.1 | 52 |
| 36 | Stability Mechanisms of Laccase Isoforms using a Modified FoldX Protocol Applicable to Widely Different Proteins. Journal of Chemical Theory and Computation, 2013, 9, 3210-3223. | 2.3 | 51 |

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| 37 | Conversion of Homocysteine to Methionine by Methionine Synthase: A Density Functional Study. Journal of the American Chemical Society, 2003, 125, 13970-13971. | 6.6 | 50 |
| 38 | Towards a â€œGolden Standardâ€•for computing globin stability: Stability and structure sensitivity of myoglobin mutants. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1239-1248. | 1.1 | 50 |
| 39 | The Influence of Selection for Protein Stability on dN/dS Estimations. Genome Biology and Evolution, 2014, 6, 2956-2967. | 1.1 | 49 |
| 40 | Electronic Structure of Cob(I)alamin:Â The Story of an Unusual Nucleophile. Journal of Physical Chemistry B, 2005, 109, 10505-10512. | 1.2 | 48 |
| 41 | Loss of stability and hydrophobicity of presenilin 1 mutations causing Alzheimer's disease. Journal of Neurochemistry, 2016, 137, 101-111. | 2.1 | 47 |
| 42 | Stability Mechanisms of a Thermophilic Laccase Probed by Molecular Dynamics. PLoS ONE, 2013, 8, e61985. | 1.1 | 46 |
| 43 | Heme: From quantum spin crossover to oxygen manager of life. Coordination Chemistry Reviews, 2017, 344, 363-374. | 9.5 | 45 |
| 44 | Molecular Mechanism of Alternative P450-Catalyzed Metabolism of Environmental Phenolic Endocrine-Disrupting Chemicals. Environmental Science & Technology, 2018, 52, 4422-4431. | 4.6 | 43 |
| 45 | The reaction mechanism of iron and manganese superoxide dismutases studied by theoretical calculations. Journal of Computational Chemistry, 2006, 27, 1398-1414. | 1.5 | 42 |
| 46 | Peroxo-Type Intermediates in Class I Ribonucleotide Reductase and Related Binuclear Non-Heme Iron Enzymes. Journal of the American Chemical Society, 2009, 131, 12155-12171. | 6.6 | 41 |
| 47 | Effect of Distal Interactions on O<sub>2</sub> Binding to Heme. Journal of Physical Chemistry B, 2013, 117, 3755-3770. | 1.2 | 39 |
| 48 | Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes. ACS Catalysis, 2017, 7, 5294-5307. | 5.5 | 38 |
| 49 | AÎ²42/AÎ²40 Ratios of Presenilin 1 Mutations Correlate with Clinical Onset of Alzheimerâ€™s Disease. Journal of Alzheimer's Disease, 2018, 66, 939-945. | 1.2 | 37 |
| 50 | Systematic Investigation of the Data Set Dependency of Protein Stability Predictors. Journal of Chemical Information and Modeling, 2020, 60, 4772-4784. | 2.5 | 37 |
| 51 | Computational Biotransformation Profile of Emerging Phenolic Pollutants by Cytochromes P450: Phenol-Coupling Mechanism. Environmental Science & Technology, 2020, 54, 2902-2912. | 4.6 | 37 |
| 52 | Cryo-temperature effects on membrane protein structure and dynamics. Physical Chemistry Chemical Physics, 2020, 22, 5427-5438. | 1.3 | 35 |
| 53 | Halide Binding and Inhibition of Laccase Copper Clusters: The Role of Reorganization Energy. Inorganic Chemistry, 2015, 54, 476-483. | 1.9 | 33 |
| 54 | Computing Stability Effects of Mutations in Human Superoxide Dismutase 1. Journal of Physical Chemistry B, 2014, 118, 1799-1812. | 1.2 | 32 |

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| 55 | Molecular dynamics of C99-bound Î³-secretase reveal two binding modes with distinct compactness, stability, and active-site retention: implications for AÎ² production. Biochemical Journal, 2019, 476, 1173-1189. | 1.7 | 32 |
| 56 | Structure and Mutations of SARS-CoV-2 Spike Protein: A Focused Overview. ACS Infectious Diseases, 2022, 8, 29-58. | 1.8 | 32 |
| 57 | O<sub>2</sub> Binding to Heme is Strongly Facilitated by Nearâ€Degeneracy of Electronic States. ChemPhysChem, 2013, 14, 3551-3558. | 1.0 | 31 |
| 58 | Copper Imbalance in Alzheimerâ€™s Disease and Its Link with the Amyloid Hypothesis: Towards a Combined Clinical, Chemical, and Genetic Etiology. Journal of Alzheimer's Disease, 2021, 83, 23-41. | 1.2 | 31 |
| 59 | A Model of Proteostatic Energy Cost and Its Use in Analysis of Proteome Trends and Sequence Evolution. PLoS ONE, 2014, 9, e90504. | 1.1 | 30 |
| 60 | Importance of proximal hydrogen bonds in haem proteins. Molecular Physics, 2003, 101, 2003-2018. | 0.8 | 29 |
| 61 | Coâ€“C Dissociation of Adenosylcobalamin (Coenzyme B<sub>12</sub>): Role of Dispersion, Induction Effects, Solvent Polarity, and Relativistic and Thermal Corrections. Journal of Physical Chemistry A, 2014, 118, 7104-7117. | 1.1 | 29 |
| 62 | Setting the stage for electron transfer: Molecular basis of ABTS-binding to four laccases from Trametes versicolor at variable pH and protein oxidation state. Journal of Molecular Catalysis B: Enzymatic, 2014, 100, 68-77. | 1.8 | 29 |
| 63 | Î²â€Amyloid pathogenesis: Chemical properties versus cellular levels. Alzheimer's and Dementia, 2016, 12, 184-194. | 0.4 | 28 |
| 64 | A base measure of precision for protein stability predictors: structural sensitivity. BMC Bioinformatics, 2021, 22, 88. | 1.2 | 28 |
| 65 | Erratum to â€œO2-binding to heme: electronic structure and spectrum of oxyheme, studied by multiconfigurational methodsâ€•[J. Inorg. Biochem. 99(1) (2004) 45â€“54]. Journal of Inorganic Biochemistry, 2005, 99, 978. | 1.5 | 27 |
| 66 | Computational studies of modified [Fe3S4] clusters: Why iron is optimal. Journal of Inorganic Biochemistry, 2008, 102, 87-100. | 1.5 | 27 |
| 67 | Improved Interaction Potentials for Charged Residues in Proteins. Journal of Physical Chemistry B, 2008, 112, 1820-1827. | 1.2 | 27 |
| 68 | The ground states of iron(III) porphines: Role of entropyâ€“enthalpy compensation, Fermi correlation, dispersion, and zero-point energies. Journal of Inorganic Biochemistry, 2011, 105, 1286-1292. | 1.5 | 26 |
| 69 | The Metal Hydride Problem of Computational Chemistry: Origins and Consequences. Journal of Physical Chemistry A, 2019, 123, 2888-2900. | 1.1 | 26 |
| 70 | Metalâ^'Ligand Bonds of Second- and Third-Row d-Block Metals Characterized by Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 10133-10141. | 1.1 | 25 |
| 71 | Structure and dynamics of Î³-secretase with presenilin 2 compared to presenilin 1. RSC Advances, 2019, 9, 20901-20916. | 1.7 | 24 |
| 72 | Insights into membrane-bound presenilin 2 from all-atom molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3196-3210. | 2.0 | 24 |

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| 73 | Rational Design of a New Trypanosoma rangeli Trans-Sialidase for Efficient Sialylation of Glycans. PLoS ONE, 2014, 9, e83902. | 1.1 | 23 |
| 74 | Modeling the Aggregation Propensity and Toxicity of Amyloid-Î² Variants. Journal of Alzheimer's Disease, 2015, 47, 215-229. | 1.2 | 23 |
| 75 | Genotype-Property Patient-Phenotype Relations Suggest that Proteome Exhaustion Can Cause Amyotrophic Lateral Sclerosis. PLoS ONE, 2015, 10, e0118649. | 1.1 | 23 |
| 76 | Benchmarking Density Functionals for Chemical Bonds of Gold. Journal of Physical Chemistry A, 2017, 121, 2022-2034. | 1.1 | 23 |
| 77 | A quantitative model of human neurodegenerative diseases involving protein aggregation. Neurobiology of Aging, 2019, 80, 46-55. | 1.5 | 23 |
| 78 | Side-by-side comparison of Notch- and C83 binding to Î³-secretase in a complete membrane model at physiological temperature. RSC Advances, 2020, 10, 31215-31232. | 1.7 | 21 |
| 79 | Three Simple Properties Explain Protein Stability Change upon Mutation. Journal of Chemical Information and Modeling, 2021, 61, 1981-1988. | 2.5 | 21 |
| 80 | Comparison of chemical properties of iron, cobalt, and nickel porphyrins, corrins, and hydrocorphins. Journal of Porphyrins and Phthalocyanines, 2005, 09, 581-606. | 0.4 | 20 |
| 81 | Bridging the gap between chemistry, physiology, and evolution: Quantifying the functionality of sperm whale myoglobin mutants. Comparative Biochemistry and Physiology Part A, Molecular & Integrative Physiology, 2012, 161, 9-17. | 0.8 | 19 |
| 82 | TtMCO: A highly thermostable laccase-like multicopper oxidase from the thermophilic Thermobaculum terrenum. Journal of Molecular Catalysis B: Enzymatic, 2015, 112, 59-65. | 1.8 | 19 |
| 83 | Trends in Strong Chemical Bonding in C<sub>2</sub>, CN, CN<sup>â€“</sup>, CO, N<sub>2</sub>, NO, NO<sup>+</sup>, and O<sub>2</sub>. Journal of Physical Chemistry A, 2017, 121, 9092-9098. | 1.1 | 19 |
| 84 | Molecular Recipe for Î³-Secretase Modulation from Computational Analysis of 60 Active Compounds. ACS Omega, 2018, 3, 18078-18088. | 1.6 | 19 |
| 85 | Computing the Pathogenicity of Alzheimerâ€™s Disease Presenilin 1 Mutations. Journal of Chemical Information and Modeling, 2019, 59, 858-870. | 2.5 | 19 |
| 86 | Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computationalâ€“Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate. Environmental Science & Technology, 2021, 55, 14037-14050. | 4.6 | 19 |
| 87 | Energy vs. density on paths toward more exact density functionals. Physical Chemistry Chemical Physics, 2018, 20, 7538-7548. | 1.3 | 18 |
| 88 | A computer-simulated mechanism of familial Alzheimerâ€™s disease: Mutations enhance thermal dynamics and favor looser substrate-binding to Î³-secretase. Journal of Structural Biology, 2020, 212, 107648. | 1.3 | 18 |
| 89 | The allyl radical revisited: a theoretical study of the electronic spectrum. Chemical Physics Letters, 2003, 380, 689-698. | 1.2 | 17 |
| 90 | The Pathogenic A2V Mutant Exhibits Distinct Aggregation Kinetics, Metal Site Structure, and Metal Exchange of the Cu<sup>2+</sup>â€“AÎ² Complex. Chemistry - A European Journal, 2017, 23, 13591-13595. | 1.7 | 17 |

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| 91 | Cell size effects in the molecular dynamics of the intrinsically disordered AÎ² peptide. Journal of Chemical Physics, 2019, 151, 085101. | 1.2 | 17 |
| 92 | Unfolding Simulations of Holomyoglobin from Four Mammals: Identification of Intermediates and Î²-Sheet Formation from Partially Unfolded States. PLoS ONE, 2013, 8, e80308. | 1.1 | 17 |
| 93 | Data set and fitting dependencies when estimating protein mutant stability: Toward simple, balanced, and interpretable models. Journal of Computational Chemistry, 2022, 43, 504-518. | 1.5 | 17 |
| 94 | Computational Chemistry of Modified [MFe<sub>3</sub>S<sub>4</sub>] and [M<sub>2</sub>Fe<sub>2</sub>S<sub>4</sub>] Clusters: Assessment of Trends in Electronic Structure and Properties. Journal of Physical Chemistry A, 2008, 112, 12829-12841. | 1.1 | 16 |
| 95 | Characterization of Sodium Stibogluconate by Online Liquid Separation Cell Technology Monitored by ICPMS and ESMS and Computational Chemistry. Analytical Chemistry, 2008, 80, 5993-6000. | 3.2 | 16 |
| 96 | Direct Correlation of Cell Toxicity to Conformational Ensembles of Genetic AÎ² Variants. ACS Chemical Neuroscience, 2015, 6, 1990-1996. | 1.7 | 16 |
| 97 | Superoxide dismutase 1 is positively selected to minimize protein aggregation in great apes. Cellular and Molecular Life Sciences, 2017, 74, 3023-3037. | 2.4 | 16 |
| 98 | Full quantum-mechanical structure of the human protein Metallothionein-2. Journal of Inorganic Biochemistry, 2012, 107, 15-24. | 1.5 | 15 |
| 99 | Ironâ€“sulfur clusters: Why iron?. Journal of Inorganic Biochemistry, 2006, 100, 1436-1439. | 1.5 | 14 |
| 100 | Accurate Computation of Reduction Potentials of 4Feâ”4S Clusters Indicates a Carboxylate Shift in Pyrococcus furiosus Ferredoxin. Inorganic Chemistry, 2007, 46, 8710-8716. | 1.9 | 14 |
| 101 | The building blocks of metallothioneins: heterometallic Zn2+ and Cd2+ clusters from first-principles calculations. Dalton Transactions, 2010, 39, 9684. | 1.6 | 14 |
| 102 | Heme isomers substantially affect heme's electronic structure and function. Physical Chemistry Chemical Physics, 2017, 19, 22355-22362. | 1.3 | 14 |
| 103 | Thermochemically Consistent Free Energies of Hydration for Di- and Trivalent Metal Ions. Journal of Physical Chemistry A, 2018, 122, 7464-7471. | 1.1 | 14 |
| 104 | Semi-empirical studies of cobalamins, corrin models, and cobaloximes. The nucleotide loop does not strain the corrin ring in cobalamins. Inorganica Chimica Acta, 2001, 323, 5-15. | 1.2 | 13 |
| 105 | Molecular dynamics derived life times of active substrate binding poses explainKMof laccase mutants. RSC Advances, 2018, 8, 36915-36926. | 1.7 | 13 |
| 106 | Computational analysis of Alzheimer-causing mutations in amyloid precursor protein and presenilin 1. Archives of Biochemistry and Biophysics, 2019, 678, 108168. | 1.4 | 13 |
| 107 | Pathogenic properties of Alzheimer's Î²-amyloid identified from structureâ€“property patient-phenotype correlations. Dalton Transactions, 2015, 44, 2747-2754. | 1.6 | 12 |
| 108 | Free Energies of Hydration for Metal Ions from Heats of Vaporization. Journal of Physical Chemistry A, 2019, 123, 6536-6546. | 1.1 | 12 |

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| 109 | Survival of the cheapest: how proteome cost minimization drives evolution. Quarterly Reviews of Biophysics, 2020, 53, e7. | 2.4 | 12 |
| 110 | Accuracy of theoretical catalysis from a model of iron-catalyzed ammonia synthesis. Communications Chemistry, 2018, 1, . | 2.0 | 11 |
| 111 | Chemical Causes of Metal Nobleness. ChemPhysChem, 2020, 21, 360-369. | 1.0 | 11 |
| 112 | Assessment of AlphaFold2 for Human Proteins via Residue Solvent Exposure. Journal of Chemical Information and Modeling, 2022, 62, 3391-3400. | 2.5 | 11 |
| 113 | Electron Transfer of Hydrated Transition-Metal Ions and the Electronic State of Co3+(aq). Inorganic Chemistry, 2018, 57, 7914-7924. | 1.9 | 10 |
| 114 | Computing the Pathogenicity of Wilsonâ€™s Disease ATP7B Mutations: Implications for Disease Prevalence. Journal of Chemical Information and Modeling, 2019, 59, 5230-5243. | 2.5 | 10 |
| 115 | Membrane dynamics of Î³â€secretase with the anterior pharynxâ€defective 1B subunit. Journal of Cellular Biochemistry, 2021, 122, 69-85. | 1.2 | 10 |
| 116 | Aerobic dive limits of seals with mutant myoglobin using combined thermochemical and physiological data. Comparative Biochemistry and Physiology Part A, Molecular & Integrative Physiology, 2013, 164, 119-128. | 0.8 | 9 |
| 117 | Contribution of substrate reorganization energies of electron transfer to laccase activity. Physical Chemistry Chemical Physics, 2019, 21, 15805-15814. | 1.3 | 9 |
| 118 | Performance of Density Functional Theory for Transition Metal Oxygen Bonds. ChemPhysChem, 2019, 20, 3210-3220. | 1.0 | 9 |
| 119 | Metallothionein Zn<sup>2+</sup>- and Cu<sup>2+</sup>-clusters from first-principles calculations. Dalton Transactions, 2012, 41, 2247-2256. | 1.6 | 8 |
| 120 | Understanding familial Alzheimer's disease: The fitâ€stayâ€trim mechanism of Î³â€secretase. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1556. | 6.2 | 8 |
| 121 | Experimentally calibrated computational chemistry of tryptophan hydroxylase: Trans influence, hydrogen-bonding, and 18-electron rule govern O2-activation. Journal of Inorganic Biochemistry, 2010, 104, 136-145. | 1.5 | 7 |
| 122 | Redox Potentials and Electronic States of Iron Porphyrin IX Adsorbed on Single Crystal Gold Electrode Surfaces. Langmuir, 2018, 34, 3610-3618. | 1.6 | 7 |
| 123 | Bioinorganic Chemistry of Zinc in Relation to the Immune System. ChemBioChem, 2022, 23, . | 1.3 | 7 |
| 124 | Identification of Structural Calcium Binding Sites in Membrane-Bound Presenilin 1 and 2. Journal of Physical Chemistry B, 2020, 124, 4697-4711. | 1.2 | 6 |
| 125 | Computational prediction and molecular mechanism of Î³-secretase modulators. European Journal of Pharmaceutical Sciences, 2021, 157, 105626. | 1.9 | 6 |
| 126 | Using electronegativity and hardness to test density functionals. Journal of Chemical Physics, 2020, 152, 244113. | 1.2 | 5 |

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| 127 | Tracking evolution of myoglobin stability in cetaceans using experimentally calibrated computational methods that account for generic protein relaxation. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2016, 1864, 825-834. | 1.1 | 4 |
| 128 | Common mechanism of thermostability in small Î±â€•and Î²â€proteins studied by molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1233-1250. | 1.5 | 4 |
| 129 | Mutants of Micromonospora viridifaciens sialidase have highly variable activities on natural and non-natural substrates. Protein Engineering, Design and Selection, 2015, 28, 37-44. | 1.0 | 3 |
| 130 | ALS/FTD: Evolution, Aging, and Cellular Metabolic Exhaustion. Frontiers in Neurology, 2022, 13, . | 1.1 | 3 |
| 131 | The Electronic Determinants of Spin Crossover Described by Density Functional Theory. Challenges and Advances in Computational Chemistry and Physics, 2019, , 1-33. | 0.6 | 2 |
| 132 | Dioxygen Binding to all 3d, 4d, and 5d Transition Metals from Coupledâ€Cluster Theory. ChemPhysChem, 2020, 21, 2173-2186. | 1.0 | 2 |